

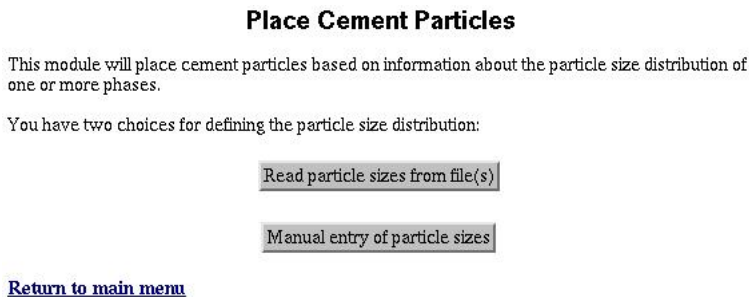
# 1 Generate initial microstructure

This submenu is used to create an initial 3-D cement paste microstructure consisting of particles of cement, gypsum, and other selected compounds in water. The user may select the amount and form of gypsum, the particle size distribution, the presence or absence of flocculation in the paste, and the presence or absence of an aggregate “slab” in the system.

**NOTE:** The microstructure image created by this submenu is composed of single-phase particles only. For example, all cement particles are assigned to be  $C_3S$  (no  $C_2S$ ,  $C_3A$ , or  $C_4AF$  is present), and any fly ash particles are supposed to be a non-descript “fly ash” phase. The distribution of phases among cement and fly ash particles is accomplished using the submenus named **Distribute cement phases** and **Distribute fly ash phases**, respectively.

Entering this submenu leads to a page shown in Figure 1. The user is asked to select how the particle size distribution is to be specified. Under usual circumstances, the user already will have created a PSD file for this purpose. In this case, the button named “Read particle sizes from file(s)” should be selected. Otherwise, if the user wishes to manually type the numbers of particles of each possible size class, then the button named “Manual entry of particle sizes” should be selected. Either way, the only difference is that, if manual entry is selected, a long table is present for typing the numbers of particles of each size for each component, and for specifying the size and resolution of the system (see the **Create a PSD File** submenu). Manual entry of particle sizes requires this table. If the user chooses to “Read particle sizes from file(s)”, then the manual entry table will be absent and the form will be considerably shorter.

**NOTE:** It is **strongly** recommended that microstructures be created from previously-defined PSD files rather than manual entry. Manual entry is tedious and prone to typographical errors that may go undetected.



**Place Cement Particles**

This module will place cement particles based on information about the particle size distribution of one or more phases.

You have two choices for defining the particle size distribution:

[Return to main menu](#)

**Figure 1:** Entry page for creating an initial 3-D microstructure.

## 1.1 Read particle sizes from files(s)

The form generated is shown in Figure 2 (top of the form) and Figure 4 (bottom of the form).

## 1.2 Random number seed

The user must enter a *negative integer*, between -32767 and -1, in this field. The random number seed is used to initiate the sequence of the C random number generator that is used in the program. Random number seeds are requested in a number of web forms, such as those for generating the microstructure, distributing clinker phases, and hydration. Choosing the same random number seed for two different runs will guarantee the same sequence of random numbers that are produced during execution of the program.

Random number seed (negative integer):

☐ [Aggregate present \(default is off\)](#) ☐ [Flocculation \(default is none\)](#)

Aggregate thickness (pixels):  Number of flocs:

[Dispersion distance between particles during placement:](#)

[Sulfate additions:](#)

Total randomly distributed calcium sulfate fraction is  with:

Hemihydrate and  Anhydrite fractions (on a total sulfate basis)

**Figure 2:** Top portion of the web form for creating an initial 3-D microstructure using pre-existing PSD files.

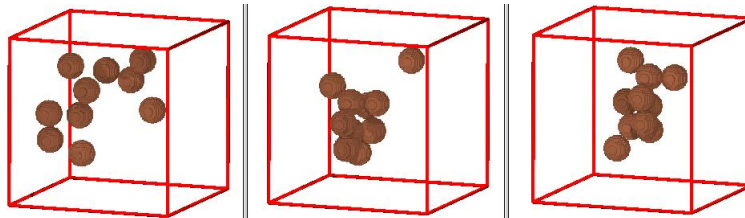
## 1.3 Aggregate present

The user may choose to place a coarse aggregate particle in the center of a 3-D microstructure. The aggregate particle is modeled as a flat plate with finite thickness. A flat-plate approximation is usually satisfactory for most applications because the surfaces of coarse aggregate particles usually have very low curvature compared to cement particles. Aggregate can be included to study the formation of the interfacial transition zone (ITZ) microstructure as a function of cement PSD, mineral admixtures, hydration, etc. The default is to exclude aggregate from the 3-D microstructure. If selected, the user should also specify the aggregate thickness (an *even integer*) for the flat plate that will be centered in the 3-D microstructure. For further information and applications on the use of aggregate slabs in computer modeling of cements, see Refs. [1, 2, 3].

## 1.4 Flocculation

The user may flocculate the cement particles after placing them in the 3-D microstructure. When a superplasticizer or high range water-reducing agent is not used, cement particles have a great tendency to flocculate together, perhaps into a single flocculated structure. Although this doesn't have a major effect on the long-term properties of hardened cement paste, it does significantly alter the rheological properties and setting behaviors of the paste. When flocculation is enabled, the user must specify the numbers of flocs to be present after flocculation. For a totally flocculated system, this value would be 1, representing a single final floc (see Figure 3 for other examples). The

default behavior is to produce no intentional flocculation, although any given particle still might be placed at random in a position of incidental contact with one or more other particles. To ensure absence of any interparticle contacts, use the **Dispersion** option described in the next paragraph. For further information, consult Refs. [4, 5, 6].



**Figure 3:** Varying degrees of flocculation among 10 equally sized cement particles. Left to right: no flocs, three flocs, and one floc.

## 1.5 Dispersion distance

When a superplasticizer or high range water-reducing agent is used, the user may elect to disperse the cement particles to model the action of these specialty chemicals. A computational trick is used to place the particles with a radius either 1 or 2 pixels larger than their true radius. Since the placed particles cannot overlap, this will assure that all particles placed are at least 1 (or 2) pixels separated from all other particles. Note that for w/c ratios below about 0.4, this dispersion may not be possible due to the large number of particles typically present in the microstructure. In this case, the program `genpartnew` will issue an error message and exit without outputting the final microstructures to file. As with flocculation, dispersion does not significantly affect the long term properties of the hydrated cement paste, but can drastically alter the rheological properties and setting behaviors. For more information, see Refs. [4, 5, 6].

**NOTE:** The user should be aware that the physical distance between dispersed particles will also depend on the chosen resolution of the system, since the resolution determines the dimension of each pixel.

## 1.6 Sulfate additions

The user has two options for placing calcium sulfate in the microstructure. If a separate PSD file for the sulfates is available, the user specifies that file later in the form. The form can even accommodate separate PSD files for the different *forms* of calcium sulfate: dihydrate, hemihydrate, and anhydrite. However, if it is assumed that the calcium sulfate and cement have the same PSD, the user may just place particles as cement and choose to have a specific volume fraction of them randomly assigned as calcium sulfate afterward. In this case, the user must input the following in the form:

- the total volume fraction of solids that is some form of calcium sulfate
- the fraction *of the total calcium sulfate* that shall be **hemihydrate**
- the fraction *of the total calcium sulfate* that shall be **anhydrite**

Particle Size Distribution Files:

Cement:	<input type="text" value="cem140wc40.psd"/>
Pozzolan:	<input type="text" value="blank.psd"/>
Fly Ash:	<input type="text" value="blank.psd"/>
Inert Filler:	<input type="text" value="blank.psd"/>
Dihydrate:	<input type="text" value="blank.psd"/>
Hemihydrate:	<input type="text" value="blank.psd"/>
Anhydrite:	<input type="text" value="blank.psd"/>

Name this microstructure:  (no file extension---.img will be added)

E-mail address:

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Please be patient, may take 3-5 minutes to execute, once you press submit.  
You will be e-mailed at the above address when execution is complete.

**Figure 4:** Bottom portion of the web form for creating an initial 3-D microstructure using pre-existing PSD files.

For example, suppose the system should have 0.02 volume fraction of dihydrate, 0.02 volume fraction of hemihydrate, and 0.01 volume fraction of anhydrite. Then the three numbers entered would be 0.05 (the sum of all three), 0.40, and 0.20, respectively. This will assign  $0.05 \times 0.40 = 0.02$  volume fraction of the placed particles as hemihydrate and  $0.05 \times 0.20 = 0.01$  volume fraction of the placed particles as anhydrite, randomly located throughout the microstructure, with the remainder (0.02) being distributed as the dihydrate form of calcium sulfate.

## 1.7 Particle size distribution files

PSD files, created using the **Create a PSD file** submenu, may be specified for several phases/compounds as shown in Figure 4. The user should note that the PSD files themselves contain only the *number* of particles of each size class to add. If more than one PSD file is specified in the form, the numbers for each size class in each file are summed. The user bears the responsibility of ensuring that the PSD files were all created in such a way as to produce the desired water-to-solids ratio.

Any of the compounds listed in Figure 4 that do *not* have an associated PSD file must have “blank.psd” entered in their field(s). For this reason, this is the default name that appears in each entry except that for cement.

Only particles  $\geq 3$  pixels in diameter are added during the particle placement routine. All one-pixel particles must be added during the specification of the hydration itself. This is done to allow the optional flocculation of the 3 pixel diameter and larger particles during the creation of the 3-D particle microstructure image. Because the 1-pixel particles are generally quite large in number, their inclusion in the flocculation algorithm would result in dramatic increases in the memory and

time requirements of the 3-D microstructure creation program.

## 1.8 Name this microstructure

The information in this web form will be used to create a microstructure “image” file that can be used in subsequent calculations or simulations. Note that only the file root should be supplied (i.e., no file extension should be added) because the VCCTL software automatically appends the extension `.img` to the name that is supplied.

## 1.9 Particle image file

When a 3-D microstructure is initially generated, *two* image files are actually created: (1) the microstructure image file itself, in which each pixel carries an integer label that specifies its phase and (2) a **particle** image file, in which each pixel carries an integer label that specifies the particle to which each pixel belongs (these latter labels range from 1 to the number of particles in the image). The particle image file is used in subsequent calculations to determine percolation properties during hydration [7] and, in some cases, to distribute fly ash phases on a particle basis. The name for the particle image file is automatically generated (no user input required) by placing the character “p” at the beginning of the microstructure image file specified in the form.

## 1.10 E-mail address

Some of the calculations performed by VCCTL may take several minutes to complete. The user may enter an e-mail address to which a note will be automatically sent upon completion of the calculation. If no e-mail address is supplied, then a note will not be generated.

Again, once the user verifies that all the information on the form is correct and presses the “Submit” button, an output page is generated with all the relevant information, including the name of the microstructure image file. It is recommended that the output page be printed and kept as a record of the file name that was chosen.

## References

- [1] D.P. Bentz and E.J. Garboczi. Simulation studies of the effects of mineral admixtures on the cement paste-aggregate interfacial zone. *ACI Materials Journal*, 88:518–529, 1991. Available at <http://ciks.cbt.nist.gov/monograph/paper23/paper23.html>.
- [2] D.P. Bentz, E. Schlangen, and E.J. Garboczi. Computer simulation of interfacial zone microstructure and its effect on the properties of cement-based composites. In J.P. Skalny and S. Mindess, editors, *Materials Science of Concrete IV*, pages 155–200. American Ceramic Society, Westerville, OH, 1995.
- [3] D.P. Bentz and E.J. Garboczi. Computer modelling of interfacial transition zone microstructure and properties. In M.G. Alexander, G. Arliguie, G. Ballivy, A. Bentur, and J. Marchand,

editors, *Engineering and Transport Properties of the Interfacial Transition Zone in Cementitious Composites*, pages 349–385. RILEM, Paris, FRANCE, 1999.

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- [5] S.P. Jiang, J.C. Mutin, and A. Nonat. Studies on mechanism and physico-chemical parameters at the origin of cement setting: I. the fundamental processes involved during the cement setting. *Cement and Concrete Research*, 25(4):779–789, 1995.
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- [7] D.P. Bentz. Cemhyd3d: A three-dimensional cement hydration and microstructural development modelling package. version 2.0. NISTIR 6485, U.S. Department of Commerce, April 2000.